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On the Randić index of graphs *

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Abstract

For a given graph $G = (V, E)$, the degree mean rate of an edge $uv \in E$ is a half of the quotient between the geometric and arithmetic means of its end-vertex degrees $d(u)$ and $d(v)$. In this note, we derive tight bounds for the Randić index of G in terms of its maximum and minimum degree mean rates over its edges. As a consequence, we prove the known conjecture that the average distance is bounded above by the Randić index for graphs with order n large enough, when the minimum degree δ is greater than (approximately) $\Delta^{\frac{1}{3}}$, where Δ is the maximum degree. As a by-product, this proves that almost all random (Erdős-Rényi) graphs satisfy the conjecture.

Keywords: Edge degree rate, Randić index, connectivity index, mean distance.

MSC: 05C35, 05C90.

1 Background

We consider simple graphs $G = (V, E)$, with vertex set V and edge set E . Unless some distance parameters are considered, as in the next definitions, G is not necessarily connected, but we always assume that there are no

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isolated vertices. Given two vertices $u, v \in V$, let denote by $\text{dist}(u, v)$ the distance between u and v . The *mean distance* of G is

$$\mu(G) = \frac{1}{n(n-1)} \sum_{u,v \in V} \text{dist}(u, v).$$

Let $d(u)$ denote the degree of vertex u , and δ and Δ the minimum and maximum degree of G . The *Randić index* [9], also called connectivity index, of G is

$$R(G) = \sum_{uv \in E} \frac{1}{\sqrt{d(u)d(v)}}.$$

Fajtlowicz [6] conjectured that, for any (connected) graph G ,

$$\mu(G) \leq R(G). \quad (1)$$

Besides, Caporossi and Hansen [5] generalized this conjecture by proposing the inequality

$$\mu(G) \leq R(G) - \left[\sqrt{n-1} - 2 \left(1 - \frac{1}{n} \right) \right]. \quad (2)$$

Since then, some sufficient conditions have been given for these conjectures to hold. For instance, Li and Shi [7] proved that, for any $\epsilon \in (0, 1)$, if G has minimum degree $\delta \geq \epsilon n$, then (1) holds for order n large enough. In fact, we show that this result is a consequence of our main theorem and the following bound for $\mu(G)$ in terms of δ (see Beezer, Riegsecker, and Smith [1]).

$$\mu(G) \leq \frac{n}{\delta + 1} + 2. \quad (3)$$

2 Bounds of the Randić index for graphs with given degree mean rate

Before giving our main result, we introduce the following concept. Given a graph $G = (V, E)$, the *degree mean rate* $\gamma(e)$ of an edge $e = uv \in E$ is a half of the quotient between the geometric and arithmetic means of its end-vertex degrees $d(u)$ and $d(v)$, that is,

$$\gamma(uv) = \frac{\sqrt{d(u)d(v)}}{d(u) + d(v)} = \frac{\sqrt{\frac{d(v)}{d(u)}}}{1 + \frac{d(v)}{d(u)}}.$$

Moreover, the maximum and minimum of this parameter over all the edges of G are denoted by

$$\Delta_E = \max_{uv \in E} \gamma(uv) \quad \text{and} \quad \delta_E = \min_{uv \in E} \gamma(uv).$$

Notice that

$$\frac{\sqrt{n-1}}{n} \leq \delta_E \leq \Delta_E \leq \frac{1}{2}, \quad (4)$$

with lower and upper bounds attained, respectively, by (any edge of) the star $S_n (= K_{1,n-1})$ and a regular graph.

Theorem 2.1. *Let $G = (V, E)$ be a graph on n vertices, with given Δ_E and δ_E . Then, its Randić index $R(G)$ satisfies the following bounds:*

$$n\delta_E \leq R(G) \leq n\Delta_E. \quad (5)$$

Proof. Notice first that, as

$$\sum_{uv \in E} \left(\frac{1}{d(u)} + \frac{1}{d(v)} \right) = \frac{1}{2} \left(\sum_{u \in V} 1 + \sum_{v \in V} 1 \right) = n,$$

for any given constant, say $\rho > 0$, the Randić index can be written as

$$R(G) = \rho + \sum_{uv \in E} \left[\frac{1}{\sqrt{d(u)d(v)}} - \frac{\rho}{n} \left(\frac{1}{d(u)} + \frac{1}{d(v)} \right) \right]. \quad (6)$$

Moreover, the function

$$z = f(x, y) = \frac{1}{\sqrt{xy}} - \frac{\rho}{n} \left(\frac{1}{x} + \frac{1}{y} \right)$$

takes zero value at the straight lines with equations $y = \alpha x$ and $y = \beta x$, where

$$\alpha = \frac{\frac{n}{2}(n - \sqrt{n^2 - 4\rho^2}) - \rho^2}{\rho^2};$$

$$\beta = \frac{\frac{n}{2}(n + \sqrt{n^2 - 4\rho^2}) - \rho^2}{\rho^2} = \alpha^{-1}.$$

Figure 1 (left) shows the function $z = f(x, y)$, when $n = 20$ and $\rho = 8$, for the region of interest $1 \leq x, y \leq n - 1$. Besides, it happens that $f(x, y) \geq 0$ inside the region where $\alpha \leq \frac{y}{x} \leq \beta$ (corresponding to the regions (II) and (III) in Figure 1 (right)), and $f(x, y) \leq 0$ otherwise.

Now, let us go back to (6) by taking $x = d(u)$ and $y = d(v)$ and, without loss of generality (because of the symmetry of $f(x, y)$), assume that $d(u) \geq d(v)$. If, for some $\rho > 0$, we have

$$(1 \geq) a = \min_{uv \in E} \frac{d(v)}{d(u)} = \alpha, \quad (7)$$

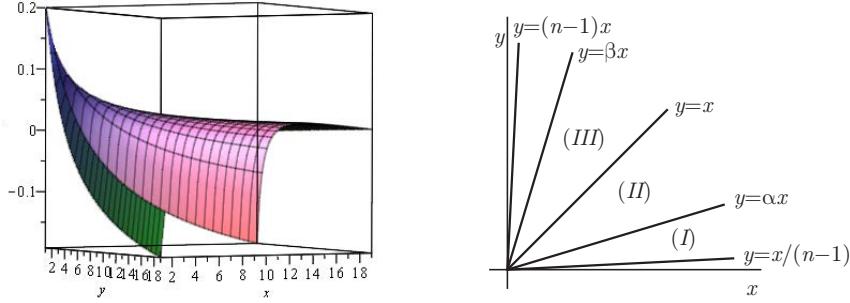


Figure 1: Left: The function $z = f(x, y)$, when $n = 20$ and $\rho = 8$, for the region of interest $1 \leq x, y \leq n-1$. Right: The different regions of $z = f(x, y)$ in the plane xy .

then all the other values of $\frac{d(v)}{d(u)}$ are inside of the cone, in the region (II) in Figure 1. Hence, $R(G) \geq \rho$. Otherwise, if, for some $\rho > 0$, we have

$$\left(\frac{1}{n-1} \leq\right) b = \max_{uv \in E} \frac{d(v)}{d(u)} = \alpha, \quad (8)$$

then all the other values of $\frac{d(v)}{d(u)}$ are outside of the cone, in the region (I) in Figure 1. Hence, $R(G) \leq \rho$. Then, solving for ρ (positive), we see that the conditions (7) and (8) are equivalent, respectively, to

$$\rho = \frac{n\sqrt{a}}{a+1} = n\delta_E; \quad (9)$$

$$\rho = \frac{n\sqrt{b}}{b+1} = n\Delta_E. \quad (10)$$

The above equalities are due to the fact that the function $\phi(x) = \frac{\sqrt{x}}{x+1}$ is increasing for $x \in (0, 1)$. Thus, the best lower and upper bounds in (5) are given, respectively, by (9) and (10). This completes the proof. \square

Note that the graphs G that satisfy $n\delta_E = R(G) = n\Delta_E$ are those whose ratio $d(v)/d(u)$ is constant for every edge. In this case, $a = b$ (see (7) and (8)), and then $\delta_E = \Delta_E = \sqrt{a}/(1+a)$ and $R(G) = n\sqrt{a}/(1+a)$. An example is given by the complete bipartite graphs K_{n_1, n_2} having $R(K_{n_1, n_2}) = \sqrt{n_1 n_2}$. Another example is provided by the trees T_p , for $p = 1, 2, \dots$, with sets of vertices V_0, V_1, \dots, V_p , such that V_0 is a singleton with degree 2^p , and every vertex of V_i (with degree 2^{p-i}) is adjacent to one vertex of V_{i-1} and $2^{p-i} - 1$ vertices of V_{i+1} . Thus, every edge of T_p , say uv with $u \in V_i$ and $v \in V_{i+1}$, has $\frac{d(v)}{d(u)} = \frac{2^{p-i-1}}{2^{p-i}} = \frac{1}{2}$, so $\delta_E = \Delta_E = \sqrt{2}/3$ and $R(T_p) = n\sqrt{2}/3$. See the example of T_3 in Figure 2 (f).

See Table 1 for the values of the Randić index and the given bounds for the graphs of Figure 2 (a)–(e).

Graph	$n\delta_E$	$R(G)$	$n\Delta_E$
(a)	5.629	5.974	6.128
(b)	2.828	2.914	3
(c)	2.449	2.710	3.5
(d)	2.904	2.957	3
(e)	2.710	2.834	2.981

Table 1: Values of $n\delta_E$, $R(G)$ and $n\Delta_E$ for the graphs of Figure 2 (a)–(e).

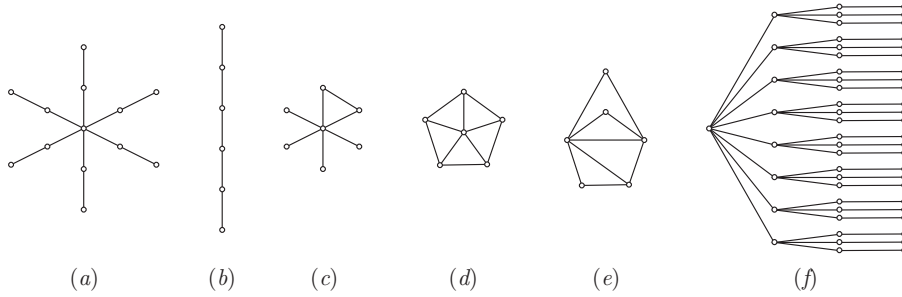


Figure 2: The graphs (a)–(e) correspond to Table 1, and (f) is the tree T_3 satisfying $n\delta_E = R(G) = n\Delta_E$.

As a corollary of Theorem 2.1, we obtain the following known result (see Bollobás and Erdős [3], or Pavlović and Gutman [8], or Caporossi, Gutman, Hansen, and Pavlović [4]).

Corollary 2.2. *The Randić index of any graph G satisfies*

$$\sqrt{n-1} \leq R(G) \leq \frac{n}{2}.$$

Moreover, the lower bound is attained if and only if $G = K_{1,n}$ (or star graph), and the upper bound is attained if and only if all components of G are regular (not necessarily with equal degree of regularity).

Proof. The lower and upper bounds come from (4). Besides, $G = K_{1,n}$ if and only if, in the proof of Theorem 2.1, $a = b = 1/(n-1)$, that is, $R(G) = n\delta_E = n\Delta_E = \sqrt{n-1}$. Analogously, all components of G are regular if and only $a = b = 1$, that is, $R(G) = n\delta_E = n\Delta_E = \frac{n}{2}$. \square

Another consequence of Theorem 2.1 is a sufficient condition for the conjecture $\mu(G) \leq R(G)$ to hold.

Corollary 2.3. *Let G be a graph with minimum degree δ satisfying*

$$\delta \geq \frac{n}{n\delta_E - 2} - 1. \quad (11)$$

Then, its Randić index satisfies $\mu(G) \leq R(G)$.

Proof. Apply Theorem 2.1 by using the bound for $\mu(G)$ in (3). \square

In particular, if $\frac{n\sqrt{\delta/\Delta}}{1+\delta/\Delta} \geq \frac{n}{\delta+1} + 2$, as $\delta_E \geq \frac{\sqrt{\delta/\Delta}}{1+\delta/\Delta}$, then we have

$$\mu(G) \leq \frac{n}{\delta+1} + 2 \leq \frac{n\sqrt{\delta/\Delta}}{1+\delta/\Delta} \leq n\delta_E \leq R(G). \quad (12)$$

So, one see that the conjecture $\mu(G) \leq R(G)$ holds, for n large enough, when δ is greater than (approximately) $\Delta^{\frac{1}{3}}$. Indeed, dividing by n the second inequality in (12), we only need to show that

$$\frac{1}{\delta+1} < \frac{\sqrt{\delta/\Delta}}{1+\delta/\Delta}$$

or, equivalently, $\sqrt{\Delta/\delta} + \sqrt{\delta/\Delta} - 1 < \delta$, which holds when $\Delta < \delta^3$ since $\delta/\Delta \leq 1$.

Moreover, Corollary 2.3 implies the result of Li and Shi [7]:

Corollary 2.4. *For any given $\epsilon \in (0, 1)$, if G is a (connected) graph with order n and minimum degree $\delta \geq \epsilon n$, then its Randić index satisfies $\mu(G) \leq R(G)$ for sufficiently large n .*

Proof. Since $\delta \geq \epsilon n$ and $\Delta \leq n-1$, we have that $\delta_E \geq \frac{\sqrt{n(n-1)\epsilon}}{n(\epsilon+1)-1}$. Then, for n large enough (for the second inequality to hold), we have

$$\delta \geq n\epsilon \geq \frac{n}{\frac{n\sqrt{n(n-1)\epsilon}}{n(\epsilon+1)-1} - 2} - 1 \geq \frac{n}{n\delta_E - 2} - 1 \quad (13)$$

and Corollary 2.3 gives the result. \square

To have an idea about the lower bound for n , notice that the second inequality in (13) gives (approximately) $n \geq \epsilon^{-3/2}$. Indeed, for large n , such inequality holds if $n\epsilon > \frac{n}{\frac{\sqrt{n(n-1)\epsilon}}{\epsilon+1}}$, that is, $\epsilon > \frac{\epsilon+1}{n\sqrt{\epsilon}}$ or $n > \epsilon^{-1/2} + \epsilon^{-3/2}$ that,

for small values of ϵ , can be approximated by $n > \epsilon^{-3/2}$, as claimed.

In Table 2 we have listed, for $\epsilon = 1/r$ and $r = 2, \dots, 20$, the bound on n given by the second inequality in (13) considering the equality, and its approximation $\epsilon^{-3/2}$. Notice that, for $\epsilon \leq 1/13$, the latter always applies.

Now we consider a random graph G from the standard Erdős-Rényi model $\mathcal{G}(n, p)$. That is, G has n vertices and each edge appears independently with probability p . Then, the condition $\delta > \Delta^{\frac{1}{3}}$ implies the following result.

ϵ	bound on n from (13)	$\epsilon^{-3/2}$
1/2	7.4	2.8
1/3	9.6	5.2
1/4	12.2	8
1/5	15.1	11.2
1/6	18.2	14.7
1/7	21.7	18.5
1/8	25.3	22.6
1/9	29.2	27
1/10	33.3	31.6
1/11	37.6	36.5
1/12	42.1	41.6
1/13	46.8	46.9
1/14	51.7	52.4
1/15	56.8	58.1
1/16	62.1	64
1/17	67.6	70.1
1/18	73.2	76.4
1/19	79	82.8
1/20	84.9	89.4

Table 2: Comparison between the bounds for n required by the second inequality in (13) when considering the equality, and its approximation $\epsilon^{-3/2}$.

Corollary 2.5. *Given any $p > 0$ almost every graph G in $\mathcal{G}(n, p)$ satisfies $\mu(G) \leq R(G)$.*

Proof. It is known that, in the Erdős-Rényi model, almost all graphs G have maximum degree

$$\Delta(G) = p(n-1) + (2pqn \log n)^{\frac{1}{2}} + o((n \log n)^{\frac{1}{2}})$$

where $q = 1 - p$. (See Bollobás [2]).

Since the minimum degree of G is $n - 1$ minus the maximum degree of the complement of G , this implies that almost all graphs G in $\mathcal{G}(n, p)$ have minimum degree

$$\begin{aligned} \delta(G) &= n - 1 - p(n-1) - (2pqn \log n)^{\frac{1}{2}} + o((n \log n)^{\frac{1}{2}}) \\ &= q(n-1) - (2pqn \log n)^{\frac{1}{2}} + o((n \log n)^{\frac{1}{2}}). \end{aligned}$$

Now, the result follows from the fact that

$$\frac{\Delta(G)}{\delta(G)^3} \xrightarrow{n \rightarrow \infty} 0.$$

□

In a similar way as done for the Randić index, we could find lower and upper bounds for the *generalized Randić index*

$$R_{\alpha}(G) = \sum_{uv \in E} (d(u)d(v))^{\alpha},$$

where now α is an arbitrary real number (the standard Randić index corresponds to $\alpha = -1/2$). More precisely, the same method applies from the following equality:

$$R_{\alpha}(G) = \rho + \sum_{uv \in E} \left[(d(u)d(v))^{\alpha} - \frac{\rho}{n} \left(\frac{1}{d(u)} + \frac{1}{d(v)} \right) \right].$$

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